Propyl-d7 alcohol
102910-31-6 | DTXSID70480193

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 4.92

Global applicability domain: Inside

Local applicability domain index: 5.42e-01

Confidence level: 7.50e-01

Nearest Neighbors from the Training Set

Image not found
tert-Butyl alcohol
Measured: 5.01
Predicted: 4.48

Image not found
3-Pyridinamine
Measured: 2.09
Predicted: 3.04

Image not found
4-Aminopyridine
Measured: 4.57
Predicted: 3.04

Image not found
Diethyl ether
Measured: 5.37
Predicted: 4.72

Image not found
2-Aminopyridine
Measured: 11.5
Predicted: 3.44